

# **Spin-orbit coupling in transactinide chemistry: secondary periodicity and effects in high-symmetry ligand fields**

C.S. Nash<sup>1</sup>

<sup>1</sup> University of New England, USA

CNash@une.edu

Extreme spin-orbit coupling extant for the transactinides is known to have dramatic effects on the valence electronic structure of 6d-block and 7p-block elements. We will examine the consequences of these severe spin-orbit effects on the nature of the transactinide ligand field of 6d transactinide coordination compounds and discuss their implications on their structure, bonding, and spectra vis-à-vis analogs of lower periods. In addition, we will address the question of what constitutes a closed-shell or chemically satisfied valence in light of the secondary periodicity wrought by spin-orbit effects. In particular, we will discuss the effect of spin-orbit coupling on dispersion interactions in dimers of nominally closed-shell 7p-block elements. To further this end, we introduce a modified version of the Bernardi-Boys counterpoise-correction scheme which reduces the calculated overcorrection of the basis set superposition error typical of this method at the correlated level.